Heptanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoro-

1546-95-8 | DTXSID70165670

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 4.22

Global applicability domain: Inside

Local applicability domain index: 9.44e-01

Confidence level: 6.81e-01

Nearest Neighbors from the Training Set

Image not found
Isopentyl alcohol
Measured: 4.52
Predicted: 4.24

Image not found
Butylamine
Measured: 3.61
Predicted: 4.09

Image not found
1-Pentanol
Measured: 4.69
Predicted: 4.17

Image not found
Pyrrolidine
Measured: 4.07
Predicted: 4.10

Image not found
Piperidine
Measured: 4.04
Predicted: 4.32